

NEWS IPC8 For general information regarding STN implementation of IPC 8  
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 13:27:26 ON 07 MAR 2007

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:27:41 ON 07 MAR 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 MAR 2007 HIGHEST RN 925228-12-2

DICTIONARY FILE UPDATES: 6 MAR 2007 HIGHEST RN 925228-12-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

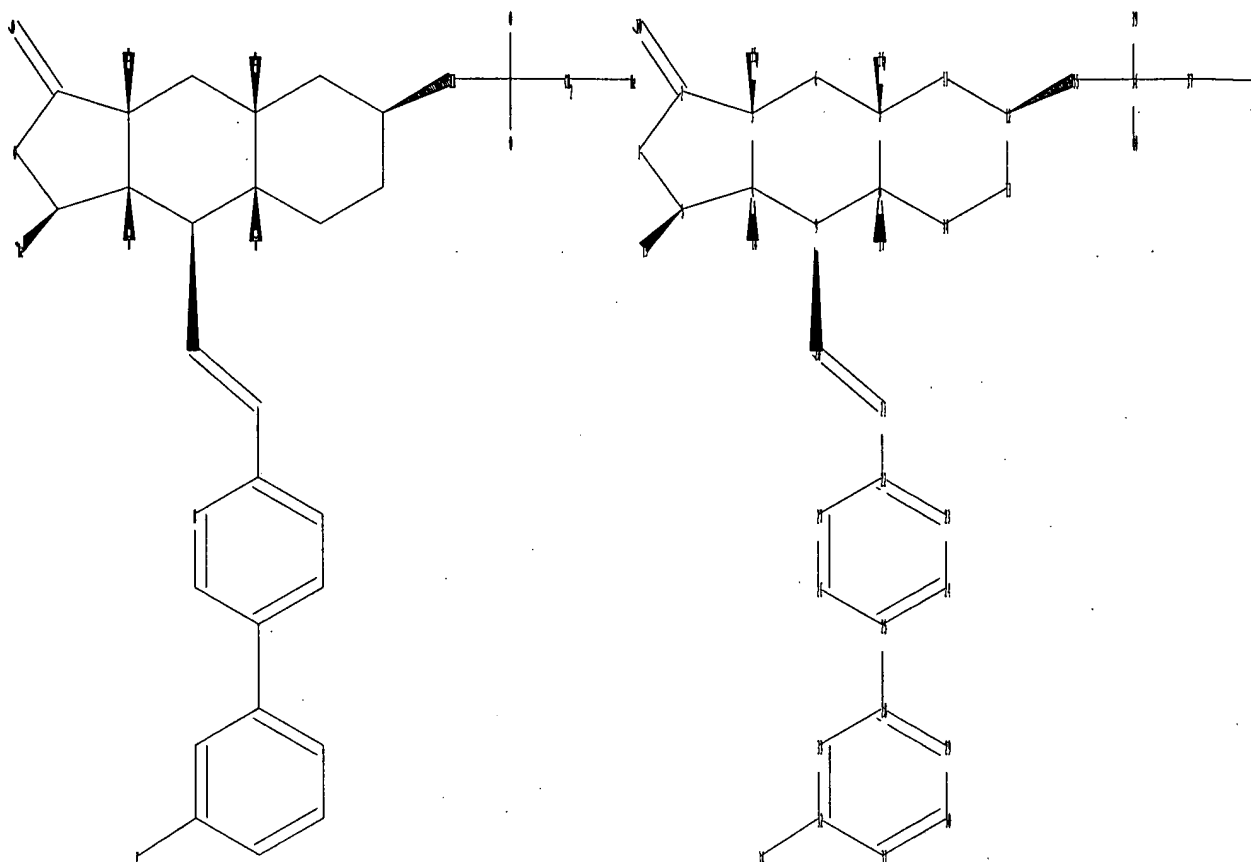
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10705282 claim 17.str



chain nodes :

38

ring nodes :

1 2 3 4 5 6 7 8 9 11 12 13 14 22 23 24 25 26 27 28 29 30 31  
32 33

ring/chain nodes :

10 15 16 17 18 19 20 21 34 35 36 37 39 40

chain bonds :

35-36 37-38

ring/chain bonds :

2-10 3-15 4-18 5-19 7-16 8-17 9-20 12-35 20-21 21-22 25-28 32-34 36-37  
36-39 36-40

ring bonds :

1-2 1-5 2-3 3-4 3-6 4-5 4-9 6-7 7-8 7-11 8-9 8-14 11-12 12-13 13-14  
22-23 22-27 23-24 24-25 25-26 26-27 28-29 28-33 29-30 30-31 31-32 32-33

exact/norm bonds :

1-2 1-5 2-3 2-10 3-4 3-6 3-15 4-5 4-9 4-18 5-19 6-7 7-8 7-11 7-16  
8-9 8-14 8-17 9-20 11-12 12-13 12-35 13-14 20-21 21-22 25-28 32-34  
35-36 36-37 36-39 36-40

exact bonds :

37-38

normalized bonds :

22-23 22-27 23-24 24-25 25-26 26-27 28-29 28-33 29-30 30-31 31-32 32-33

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom  
28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS  
37:CLASS 38:CLASS 39:CLASS 40:CLASS

Stereo Bonds:

15-3 (Single Wedge).  
16-7 (Single Wedge).  
17-8 (Single Hash).  
18-4 (Single Wedge).  
19-5 (Single Wedge).  
20-9 (Single Hash).  
35-12 (Single Hash).

Stereo Chiral Centers:

3 (Parity=Even)  
4 (Parity=Even)  
5 (Parity=Even)  
7 (Parity=Even)  
8 (Parity=Odd)  
9 (Parity=Odd)  
12 (Parity=Even)

Stereo RSS Sets:

Type=Relative (Default). 7 Nodes= 3 4 5 7 8 9 12

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 exa sam

SAMPLE SEARCH INITIATED 13:28:17 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA EXA SAM L1

=> s l1 exa full

FULL SEARCH INITIATED 13:28:22 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

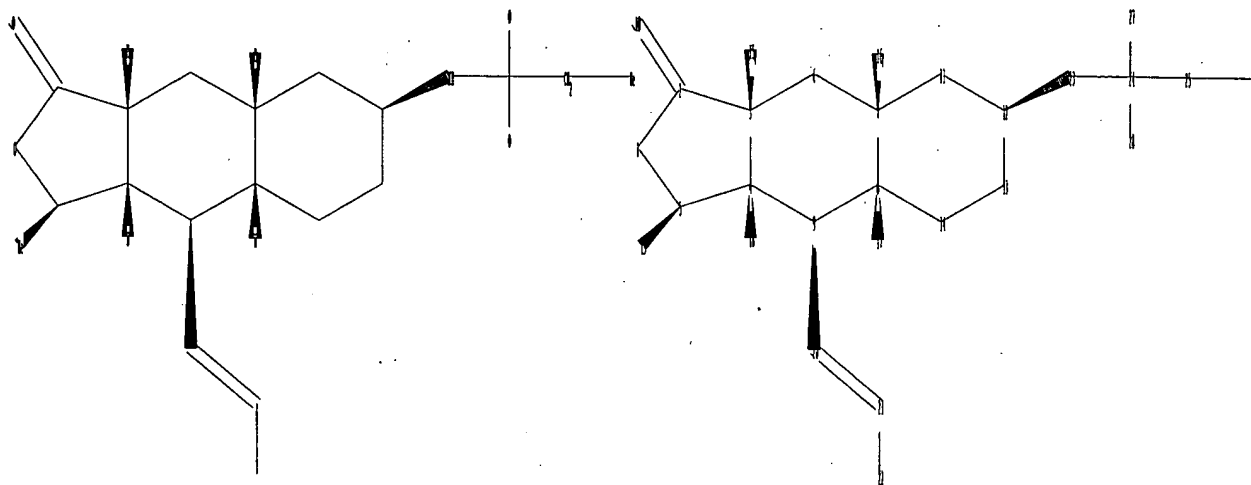
0 ANSWERS

SEARCH TIME: 00.00.01

L3 0 SEA EXA FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10705282 claim 17a.str



chain nodes :

26

ring nodes :

1 2 3 4 5 6 7 8 9 11 12 13 14

ring/chain nodes :

10 15 16 17 18 19 20 21 22 23 24 25 27 28

chain bonds :

23-24 25-26

ring/chain bonds :

2-10 3-15 4-18 5-19 7-16 8-17 9-20 12-23 20-21 21-22 24-25 24-27 24-28

ring bonds :

1-2 1-5 2-3 3-4 3-6 4-5 4-9 6-7 7-8 7-11 8-9 8-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-5 2-3 2-10 3-4 3-6 3-15 4-5 4-9 4-18 5-19 6-7 7-8 7-11 7-16

8-9 8-14 8-17 9-20 11-12 12-13 12-23 13-14 20-21 21-22 23-24 24-25

24-27 24-28

exact bonds :

25-26

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:CLASS 21:CLASS 22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS

27:CLASS 28:CLASS

Stereo Bonds:

15-3 (Single Wedge).

16-7 (Single Wedge).

17-8 (Single Hash).

18-4 (Single Wedge).

19-5 (Single Wedge).

20-9 (Single Hash).

23-12 (Single Hash).

Stereo Chiral Centers:

3 (Parity=Even)

4 (Parity=Even)

5 (Parity=Even)

7 (Parity=Even)

8 (Parity=Odd)  
9 (Parity=Odd)  
12 (Parity=Even)

Stereo RSS Sets:

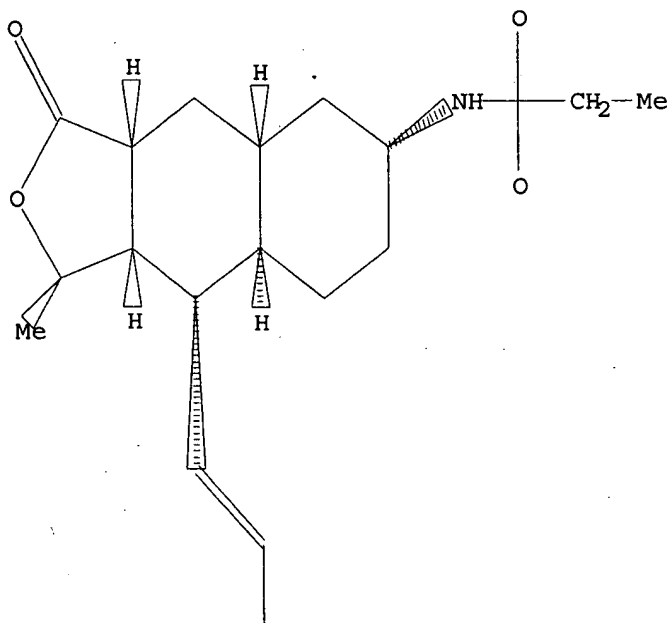
Type=Relative (Default). 7 Nodes= 3 4 5 7 8 9 12

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14 sss sam

SAMPLE SEARCH INITIATED 13:30:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 48 TO ITERATE

100.0% PROCESSED 48 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 545 TO 1375

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s 14 sss full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 13:30:33 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1000 TO ITERATE

100.0% PROCESSED 1000 ITERATIONS

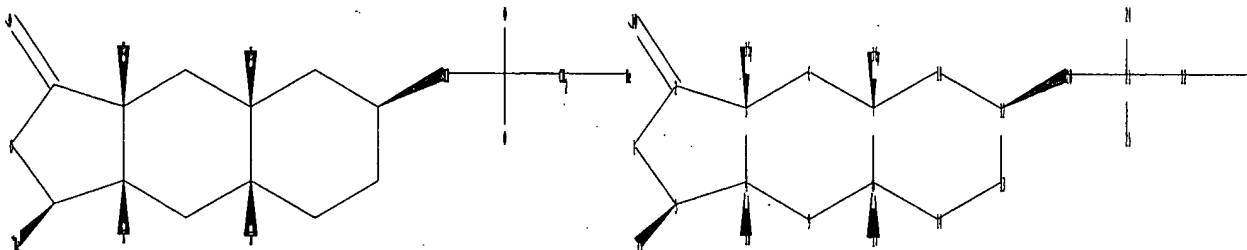
0 ANSWERS

SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>

Uploading C:\Program Files\Stnexp\Queries\10705282 claim 17b.str



chain nodes :

23

ring nodes :

1 2 3 4 5 6 7 8 9 11 12 13 14

ring/chain nodes :

10 15 16 17 18 19 20 21 22 24 25

chain bonds :

20-21 22-23

ring/chain bonds :

2-10 3-15 4-18 5-19 7-16 8-17 12-20 21-22 21-24 21-25

ring bonds :

1-2 1-5 2-3 3-4 3-6 4-5 4-9 6-7 7-8 7-11 8-9 8-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-5 2-3 2-10 3-4 3-6 3-15 4-5 4-9 4-18 5-19 6-7 7-8 7-11 7-16

8-9 8-14 8-17 11-12 12-13 12-20 13-14 20-21 21-22 21-24 21-25

exact bonds :

22-23

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

Stereo Bonds:

15-3 (Single Wedge).

16-7 (Single Wedge).

17-8 (Single Hash).

18-4 (Single Wedge).

19-5 (Single Wedge).

20-12 (Single Hash).

Stereo Chiral Centers:

3 (Parity=Even)

4 (Parity=Even)

5 (Parity=Even)

7 (Parity=Even)

8 (Parity=Odd)

12 (Parity=Even)

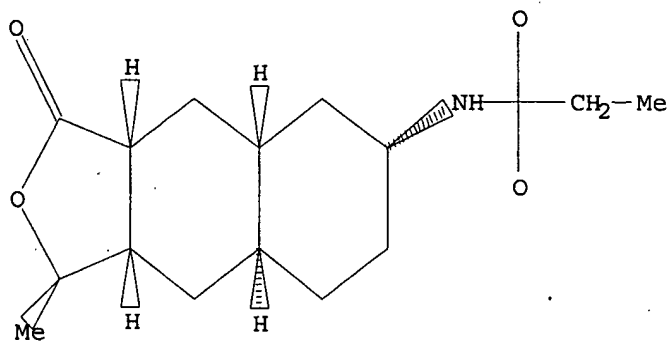
Stereo RSS Sets:

Type=Relative (Default). 6 Nodes= 3 4 5 7 8 12

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS  
L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17 sss sam

SAMPLE SEARCH INITIATED 13:32:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 48 TO ITERATE

100.0% PROCESSED      48 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH      \*\* COMPLETE \*\*

PROJECTED ITERATIONS: 545 TO 1375

PROJECTED ANSWERS: 0 TO 0

L8                    0 SEA SSS SAM L7

```
=> s 17 sss full
```

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 13:32:11 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1000 TO ITERATE

100.0% PROCESSED      1000 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

```
=> s 17 exa full
```

FULL SEARCH INITIATED 13:32:58 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED      0 ITERATIONS

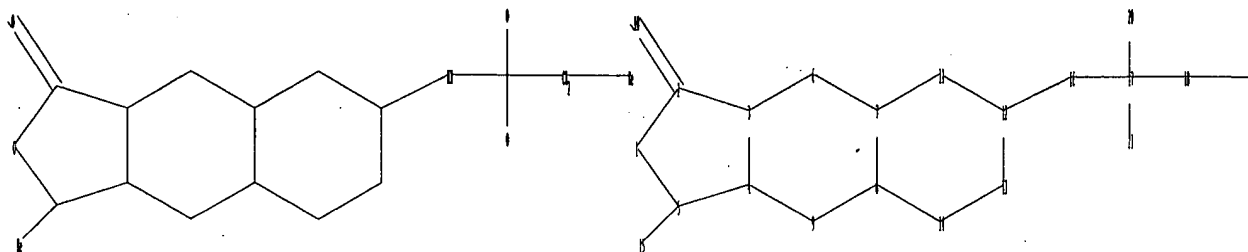
0 ANSWERS

SEARCH TIME: 00.00.01

L10                    0 SEA EXA FUL L7

 $\Rightarrow$ 

Uploading C:\Program Files\Stnexp\Queries\10705282 claim 17c.str



chain nodes :

19

ring nodes :

1 2 3 4 5 6 7 8 9 11 12 13 14

ring/chain nodes :

10 15 16 17 18 20 21

chain bonds :

5-15 16-17 18-19

ring/chain bonds :

2-10 12-16 17-18 17-20 17-21

ring bonds :

1-2 1-5 2-3 3-4 3-6 4-5 4-9 6-7 7-8 7-11 8-9 8-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-5 2-3 2-10 3-4 3-6 4-5 4-9 6-7 7-8 7-11 8-9 8-14 11-12 12-13

12-16 13-14 16-17 17-18 17-20 17-21

exact bonds :

5-15 18-19

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS

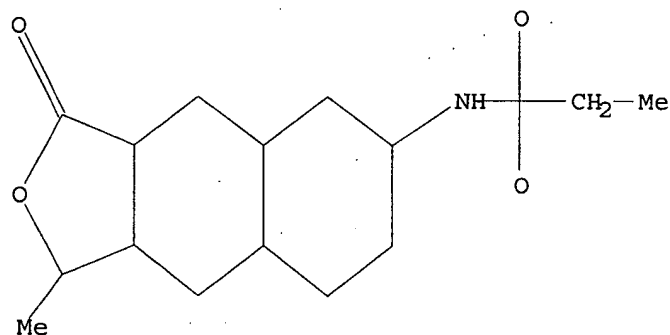
19:CLASS 20:CLASS 21:CLASS

L11 STRUCTURE UPLOADED

=> d l11

L11 HAS NO ANSWERS

L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l11 sss sam

SAMPLE SEARCH INITIATED 13:35:10 FILE 'REGISTRY'

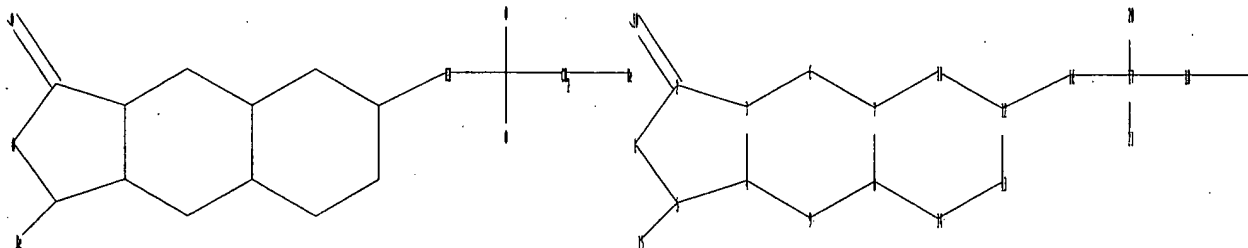


REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10705282 claim 17d.str



chain nodes :

19

ring nodes :

1 2 3 4 5 6 7 8 9 11 12 13 14

ring/chain nodes :

10 15 16 17 18 20 21

chain bonds :

16-17 18-19

ring/chain bonds :

2-10 5-15 12-16 17-18 17-20 17-21

ring bonds :

1-2 1-5 2-3 3-4 3-6 4-5 4-9 6-7 7-8 7-11 8-9 8-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-5 2-3 2-10 3-4 3-6 4-5 4-9 5-15 6-7 7-8 7-11 8-9 8-14 11-12

12-13 12-16 13-14 16-17 17-18 17-20 17-21

exact bonds :

18-19

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS

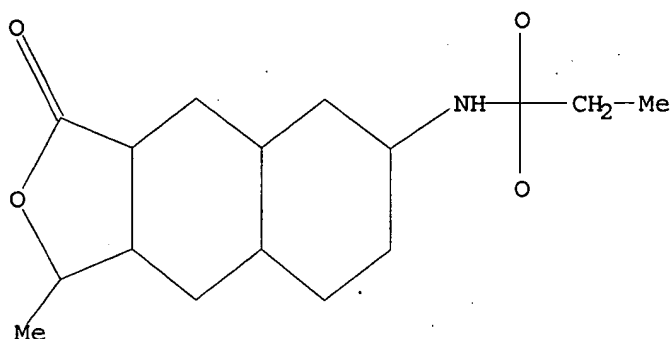
19:CLASS 20:CLASS 21:CLASS

L14 STRUCTURE UPLOADED

=> d l14

L14 HAS NO ANSWERS

L14 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l14 fam full

FULL SEARCH INITIATED 13:50:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L15 0 SEA FAM FUL L14

=> s l14

SAMPLE SEARCH INITIATED 13:51:10 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 48 TO ITERATE

100.0% PROCESSED 48 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

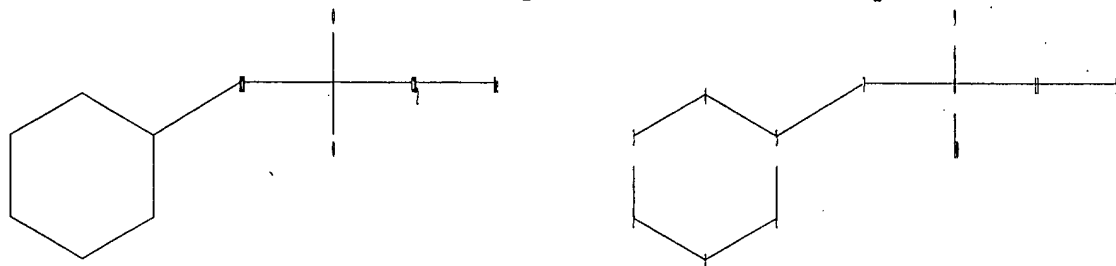
PROJECTED ITERATIONS: 545 TO 1375

PROJECTED ANSWERS: 0 TO 0

L16 0 SEA SSS SAM L14

=>

Uploading C:\Program Files\Stnexp\Queries\10705282 simple.str



chain nodes :

7 8 9 10 11 12

ring nodes :

1 2 3 4 5 6

chain bonds :

5-7 7-8 8-9 8-10 8-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 7-8 8-9 8-10

exact bonds :  
8-11 11-12

Match level :

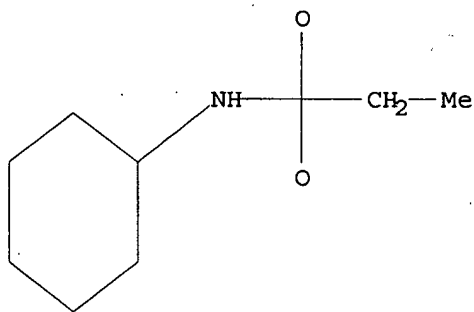
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS

L17 STRUCTURE UPLOADED

=> d 117

L17 HAS NO ANSWERS

L17 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 117 sss sam

SAMPLE SEARCH INITIATED 13:54:33 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 22 TO 418

PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> s 117 sss full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 13:54:44 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 192 TO ITERATE

100.0% PROCESSED 192 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L19 2 SEA SSS FUL L17

=> d scan

L19 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,1-Propanediol, 1-(phenylamino)-, conjugate monoacid (9CI)

MF C9 H13 N O2 . H

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT  
(Reactant); PROC (Process); RACT (Reactant or reagent)  
(MNDO study of the acid-catalyzed condensation reaction mechanism of  
propionic acid and aniline)

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

4.11

889.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.78

-0.78

FILE 'STNGUIDE' ENTERED AT 13:56:11 ON 07 MAR 2007

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Mar 2, 2007 (20070302/UP).

=> d his

(FILE 'HOME' ENTERED AT 13:27:26 ON 07 MAR 2007)

FILE 'REGISTRY' ENTERED AT 13:27:41 ON 07 MAR 2007

L1 STRUCTURE UPLOADED  
L2 0 S L1 EXA SAM  
L3 0 S L1 EXA FULL  
L4 STRUCTURE UPLOADED  
L5 0 S L4 SSS SAM  
L6 0 S L4 SSS FULL  
L7 STRUCTURE UPLOADED  
L8 0 S L7 SSS SAM  
L9 0 S L7 SSS FULL  
L10 0 S L7 EXA FULL  
L11 STRUCTURE UPLOADED  
L12 0 S L11 SSS SAM  
L13 0 S L11 SSS FULL

FILE 'REGISTRY' ENTERED AT 13:49:33 ON 07 MAR 2007

L14 STRUCTURE UPLOADED  
L15 0 S L14 FAM FULL  
L16 0 S L14  
L17 STRUCTURE UPLOADED  
L18 0 S L17 SSS SAM  
L19 2 S L17 SSS FULL

FILE 'CAPLUS' ENTERED AT 13:55:06 ON 07 MAR 2007

L20 1 S L19

FILE 'STNGUIDE' ENTERED AT 13:56:11 ON 07 MAR 2007

=>

---Logging off of STN---

=>

Executing the logoff script...